Advanced Computing Jobs:

Develop Multicore and GPU HPC Programming on SaaS Environment using Jupyter Lab

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Compilers in NVIDIA HPC SDK

nvc

nvc is a C11 compiler for NVIDIA GPUs and AMD, Intel, OpenPOWER, and Arm CPUs. It invokes the C compiler, assembler, and linker for the target processors with options derived from its command line arguments. nvc supports ISO C11, supports GPU programming with OpenACC, and supports multicore CPU programming with OpenACC and OpenMP.

nvc++

nvc++ is a C++17 compiler for NVIDIA GPUs and AMD, Intel, OpenPOWER, and Arm CPUs. It invokes the C++ compiler, assembler, and linker for the target processors with options derived from its command line arguments. nvc++ supports ISO C++17, supports GPU programming with C++17 parallel algorithms (pSTL) and OpenACC, and supports multicore CPU programming with OpenACC and OpenMP.

nvfortran

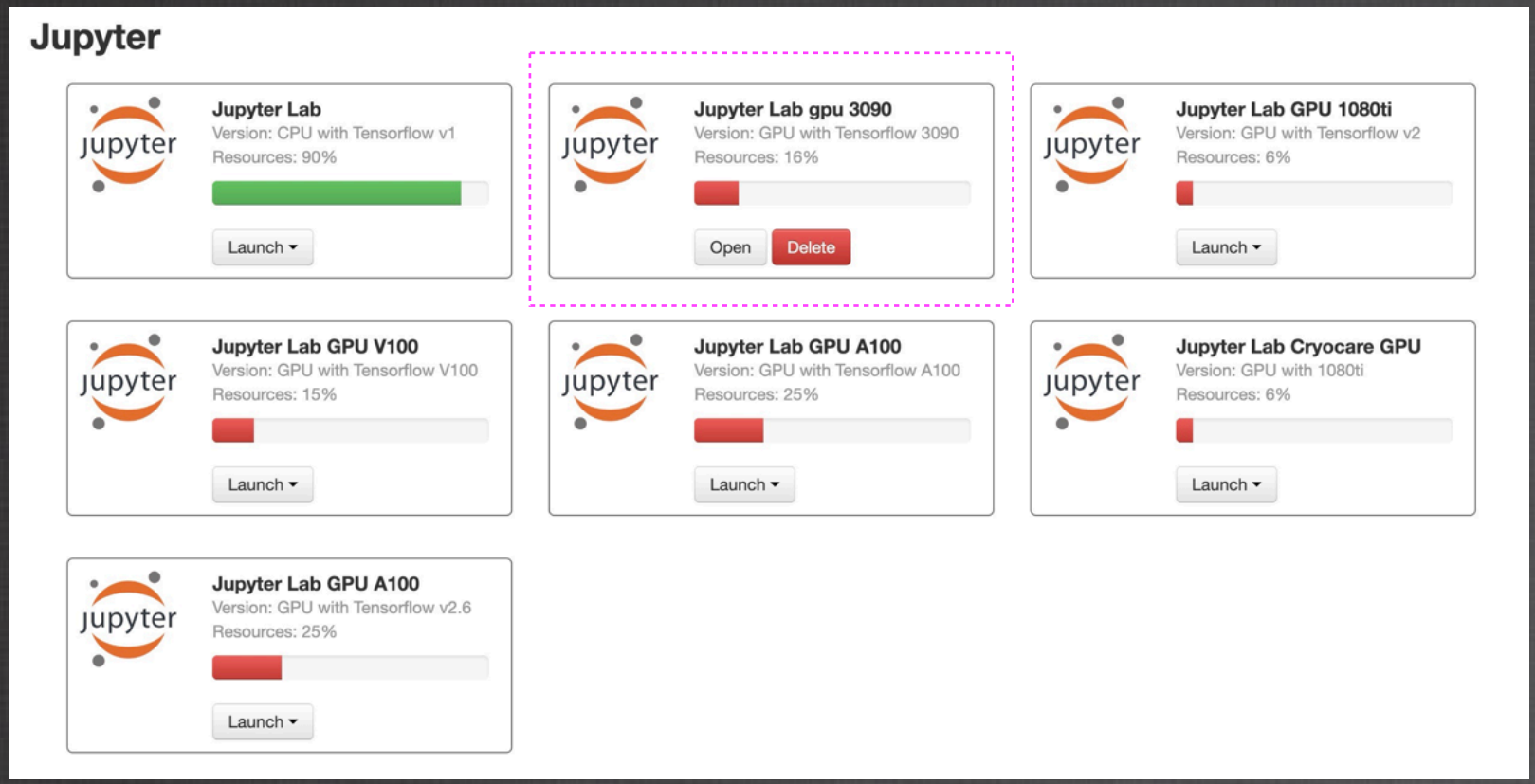
nvfortran is a Fortran compiler for NVIDIA GPUs and AMD, Intel, OpenPOWER, and Arm CPUs. It invokes the Fortran compiler, assembler, and linker for the target processors with options derived from its command line arguments. nvfortran supports ISO Fortran 2003 and many features of ISO Fortran 2008, supports GPU programming with CUDA Fortran and OpenACC, and supports multicore CPU programming with OpenACC and OpenMP.

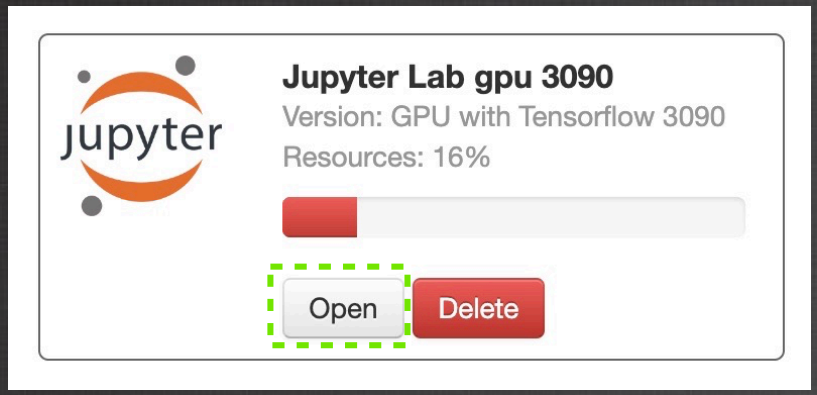
nvcc

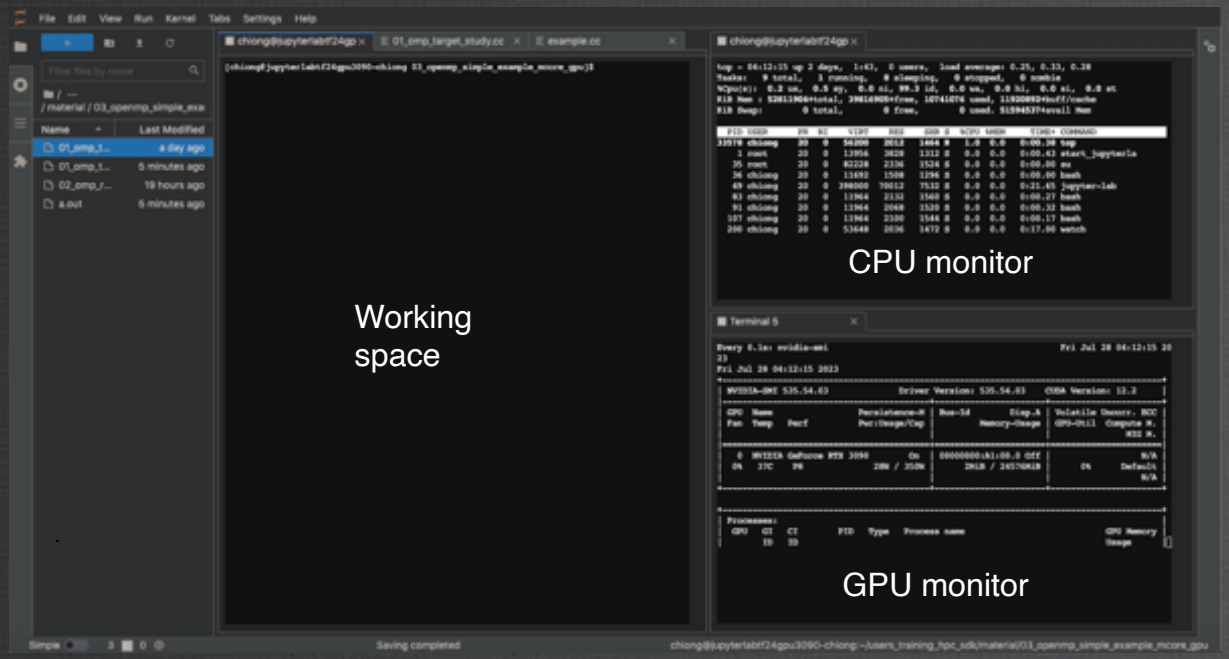
nvcc is the CUDA C and CUDA C++ compiler driver for NVIDIA GPUs. nvcc accepts a range of conventional compiler options, such as for defining macros and include/library paths, and for steering the compilation process. nvcc produces optimized code for NVIDIA GPUs and drives a supported host compiler for AMD, Intel, OpenPOWER, and Arm CPUs.

https://docs.nvidia.com/hpc-sdk/archive/20.11/index.html

https://dicos.grid.sinica.edu.tw/dockerapps/




Jupyter Lab gpu 3090
Version: GPU with Tensorflow 3090
Resources: 16%
Open
Delete


Working space
CPU monitor
GPU monitor

CPU monitor

```
top - 04:10:12 up 2 days,  1:41,  0 users,  load average: 0.60, 0.37, 0.28
Tasks:  12 total,   3 running,   9 sleeping,   0 stopped,   0 zombie
%Cpu(s):  1.4 us,  1.2 sy,  0.0 ni, 97.3 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
KiB Mem : 52811904+total, 39151625+free, 17393880 used, 11920891+buff/cache
KiB Swap:        0 total,        0 free,        0 used. 50929052+avail Mem

  PID USER      PR  NI    VIRT    RES    SHR S  %CPU %MEM     TIME+ COMMAND
36457 chiong    20   0   22.4g  16.8g   2076 R 100.0  3.3   0:03.26 a.out
36503 chiong    20   0   30796  14028   1476 R   2.0  0.0   0:00.02 nvidia-smi
  200 chiong    20   0   53648   2036   1472 S   1.0  0.0   0:16.24 watch
    1 root      20   0   13956   3828   1312 S   0.0  0.0   0:00.43 start_jupyterla
   35 root      20   0   82228   2336   1524 S   0.0  0.0   0:00.00 su
   36 chiong    20   0   11692   1508   1296 S   0.0  0.0   0:00.00 bash
   49 chiong    20   0  398000  70012   7532 S   0.0  0.0   0:21.23 jupyter-lab
   83 chiong    20   0   11964   2132   1560 S   0.0  0.0   0:00.27 bash
   91 chiong    20   0   11964   2068   1520 S   0.0  0.0   0:00.32 bash
  107 chiong    20   0   11964   2100   1544 S   0.0  0.0   0:00.17 bash
33578 chiong    20   0   56200   2012   1464 R   0.0  0.0   0:00.26 top
36502 chiong    20   0   53648    564      0 S   0.0  0.0   0:00.00 watch
```

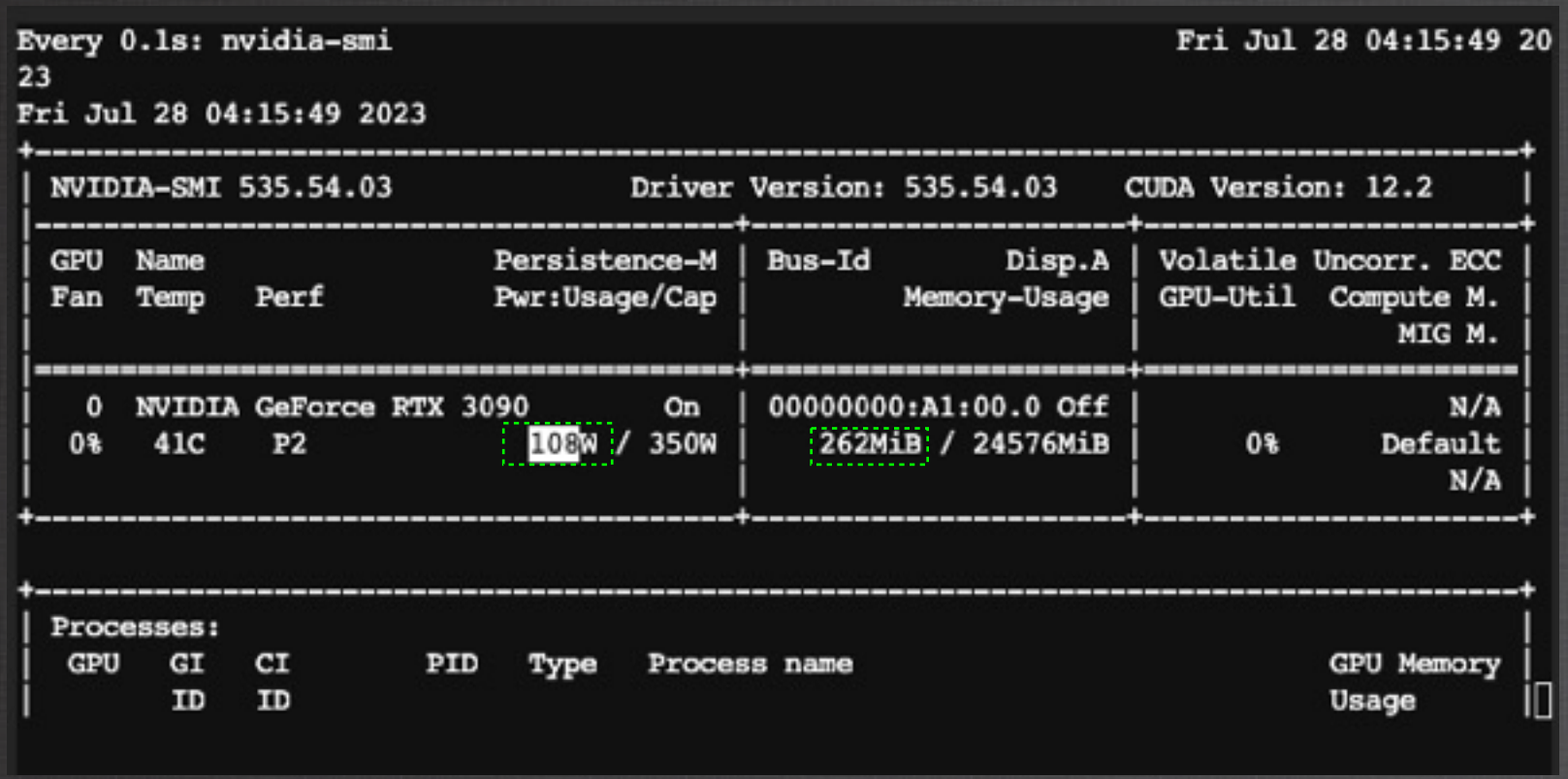
single core job

```
top - 04:08:10 up 2 days,  1:39,  0 users,  load average: 0.29, 0.23, 0.23
Tasks:  10 total,   2 running,   8 sleeping,   0 stopped,   0 zombie
%Cpu(s): 12.1 us,  2.8 sy,  0.0 ni, 85.1 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
KiB Mem : 52811904+total, 37466662+free, 34243472 used, 11920894+buff/cache
KiB Swap:        0 total,        0 free,        0 used. 49245321+avail Mem

  PID USER      PR  NI    VIRT    RES    SHR S  %CPU %MEM     TIME+ COMMAND
34663 chiong    20   0   22.8g  22.4g   2128 R 704.0  4.4   0:19.59 a.out
33578 chiong    20   0   56200   2012   1464 R   1.0  0.0   0:00.12 top
    1 root      20   0   13956   3828   1312 S   0.0  0.0   0:00.43 start_jupyterla
   35 root      20   0   82228   2336   1524 S   0.0  0.0   0:00.00 su
   36 chiong    20   0   11692   1508   1296 S   0.0  0.0   0:00.00 bash
   49 chiong    20   0  398000  70012   7532 S   0.0  0.0   0:20.80 jupyter-lab
   83 chiong    20   0   11964   2132   1560 S   0.0  0.0   0:00.26 bash
   91 chiong    20   0   11964   2068   1520 S   0.0  0.0   0:00.32 bash
  107 chiong    20   0   11964   2100   1544 S   0.0  0.0   0:00.17 bash
  200 chiong    20   0   53648   2036   1472 S   0.0  0.0   0:15.49 watch
```

multicore job
cpu usage > 100%

GPU monitor


Every 0.1s: nvidia-smi
Fri Jul 28 04:15:49 20
23
Fri Jul 28 04:15:49 2023
NVIDIA-SMI 535.54.03
Driver Version: 535.54.03
CUDA Version: 12.2
GPU Name
Fan Temp Perf
Persistence-M
Pwr:Usage/Cap
Bus-Id
Disp.A
Memory-Usage
Volatile Uncorr. ECC
GPU-Util Compute M.
MIG M.
0 NVIDIA GeForce RTX 3090
On
0% 41C P2
108W / 350W
00000000:A1:00.0 Off
262MiB / 24576MiB
N/A
0%
Default
N/A
Processes:
GPU GI CI
ID ID
PID
Type
Process name
GPU Memory
Usage

Modern C++ new features for Parallel computing

Algorithms and execution policies

Basic for-loop

```
for (Index_t i = 0; i < data.size(r); ++i)
{

}
```

Parallel algorithm for-loop running on Multicore or GPU

```
 std::for_each_n(std::execution::par, counting_iterator(0),data.size(r),
 [=, &domain](Index_t i)
{

 }
);
```

To download examples source code:

git clone https://github.com/ASGCOPS/Advanced_Computing_Job_2023
cd Advanced_Computing_Job_2023
unzip HPC_src.zip
cd material

```
01_c_plus_plus_simple_example_mcore_gpu  03_openmp_simple_example_mcore_gpu
02_c_plus_plus_LULESH_mcore_gpu          04_fortran_90_AutoPar
```

Simple code for multicore and GPU

```cpp
#include <vector>
#include <iostream>
#include <fstream>
#include <random>
#include <string>

#include <algorithm>
#include <execution>

int main()
{
int N=4000;

std::vector<int> random_number;

// Create random value vector by CPU on system memory.
for (int x=0;x<N;x++)
{
    int random_int;
    random_int=rand() % 90000;
    random_number.push_back(random_int);
}

// Sort random number with MCORE or GPU.
std::sort(std::execution::par, random_number.begin(),
random_number.end());

// Print the sort result on screen.
for (int i=0;i<20;i++)
{
    std::cout<<random_number[i]<<std::endl;
}

}
```

include files for C++17

Running on single core CPU
cpu usage ≤ 100%

Running on multicore CPU
cpu usage > 100%

To compile the code and run :

(1) Setup the NVIDIA HPC SDK envirnoment:
source /cvmfs/cvmfs.grid.sinica.edu.tw/hpc/nvhpc_sdk/2021_217/setup.sh

(2) Change your working directory:
cd 01_c_plus_plus_simple_example_mcore_gpu

(3) Compile source code for multicore:
nvc++ -stdpar=multicore example.cc

(4) Or compile source code for GPU:
nvc++ -gpu=cc80 -stdpar=gpu example.cc

(5) run
./a.out

For GPU A100 and RTX3090, the GPU capability is cc80

Larger example: LULESH

https://github.com/LLNL/LULESH/tree/2.0.2-dev/stdpar

C++ Algorithms / Policies in LULESH

```
std::for_each_n(std::execution::par, counting_iterator(0), numElem,
                [=, &domain](Index_t i) {
                  sigxx[i] = sigyy[i] = sigzz[i] = -domain.p(i) - domain.q(i);
                });
```

```
  std::for_each(std::execution::par, domain.symmX_begin(),
                domain.symmX_begin() + numNodeBC, [&domain](Index_t symmX) {
                  domain.xdd(symmX) = Real_t(0.0);
                });
```

```
std::transform(std::execution::par, compression, compression + length, bvc,
               [=](Real_t compression_i) {
                 return cls * (compression_i + Real_t(1.0));
               });
```

To compile the code and run :

(1) Setup the NVIDIA HPC SDK envirnoment:
source /cvmfs/cvmfs.grid.sinica.edu.tw/hpc/nvhpc_sdk/2021_217/setup.sh

(2) Change your working directory:
cd 02_c_plus_plus_LULUSH_mcore_gpu/build

(3) Edit the Makefile:

For multicore:
CXXFLAGS = -w -fast -Mnouniform -Mfprelaxed -stdpar=multicore -std=c++11 -DUSE_MPI=0

For GPU:
CXXFLAGS = -w -fast -Mnouniform -Mfprelaxed -stdpar=gpu -std=c++11 -DUSE_MPI=0

(4) Compile
make clean
make all

(5) Run
./lulesh2.0

Makefile

```
# Build with nvc++, with parallel algorithm support turned on.

SHELL = /bin/sh
.SUFFIXES: .cc .o

LULESH_EXEC = lulesh2.0

CXX = nvc++

SOURCES2.0 = \
  lulesh.cc \
  lulesh-comm.cc \
  lulesh-viz.cc \
  lulesh-util.cc \
  lulesh-init.cc
OBJECTS2.0 = $(SOURCES2.0:.cc=.o)


CXXFLAGS = -w -fast -Mnouniform -Mfprelaxed -stdpar=multicore -std=c++11 -DUSE_MPI=0

```

OpenMP for MCORE / GPU

Basic For-loop

```
for (Index_t i = 0; i < data.size(r); ++i)
{

}
```

OpenMP Directive

```
#pragma omp target teams distribute parallel for
for (Index_t i = 0; i < data.size(r); ++i)
{

}
```

Simple OpenMP example

```
1  #include<stdio.h>
2  #include <stdlib.h>
3
4  using namespace std;
5
6  #define N 2000000000
7
8  int main()
9  {
10   //Single core or CPU session :
11       int* a = (int*)malloc(sizeof(int) * N);
12       int* b = (int*)malloc(sizeof(int) * N);
13       int* c = (int*)malloc(sizeof(int) * N);
14
15       for (int i = 0; i < N; i++)
16       {
17               a[i] = 9;
18               b[i] = 1;
19               c[i] = 0;                    CPU
20       }
21
22
23     // Multi-core or GPU session :
24     #pragma omp target device(0) map(to: a[0:N-1]) map(to: b[0:N-1])
   map(from: c[0:N-1])
25       {                                    GPU
26
27       #pragma omp teams distribute parallel for
28       for (int i = 0; i < N; i++)
29               c[i] += a[i] + b[i];
30
31
32       }
33 }
```

Initialize arrays by single core cpu
cpu usage ≤ 100%

Calculate by multicore cpu
cpu usage > 100%

Transfer data to GPU memory
map(to: a[0:N-1])

Calculate c[i] += a[i] +b[i] on GPU

Get result from GPU memory
map(from: c[0:N-1])

To compile the code and run :

(1) Setup the NVIDIA HPC SDK envirnoment:
```
source /cvmfs/cvmfs.grid.sinica.edu.tw/hpc/nvhpc_sdk/2021_217/setup.sh
```

(2) Change your working directory:
```
cd 03_openmp_simple_example_mcore_gpu
```

(3) Compile source code for multicore:
```
nvc++ -stdpar=multicore 01_omp_target_study.cc
```

(4) Or compile source code for GPU:
```
nvc++ -gpu=cc80 -stdpar=gpu 01_omp_target_study.cc
```

(5) run
```
./a.out
```

Simple OpenMP example

```
1  // openmp reduction test
2
3  #include <stdlib.h>
4  #include <stdio.h>
5  #include <math.h>
6
7  #define COUNT 20000000
8
9  int main()
10 {
11     int sum = 0;          // Assign an initial value on system memory.
12
13     #pragma omp teams distribute parallel for reduction(+:sum)
14     for(int i = 0;i < COUNT; i++)
15     {
16         // Edit your own formula here:
17         sum += rand() % 3;
18     }
19
20     printf("\n Sum: %d\n\n",sum);
21
22     return 0;
23 }
```

To compile the code and run :

(1) Setup the NVIDIA HPC SDK envirnoment:

```
source /cvmfs/cvmfs.grid.sinica.edu.tw/hpc/nvhpc_sdk/2021_217/setup.sh
```

(2) Change your working directory:

```
cd 03_openmp_simple_example_mcore_gpu
```

(3) Compile source code for multicore:

```
nvc++ -gpu=cc80 -stdpar=multicore 02_omp_reduction.cc
```

(4) run

```
./a.out
```